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A Computation Approach to Chance Constrained Optimization of Boundary-Value Parabolic Partial Differential Equation Systems

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Abstract: This work studies chance constrained optimization of boundary-value parabolic partial differential equations (CCPDE) with random data, where the PDE model is treated as equality constraint and chance constraints are imposed on inequality constraints involving state variables. Since such a CCPDE problem is generally non-smooth, non-convex and difficult to solve directly, we use our recently proposed smoothing approximation method to solve the problem. As a result, the probability function of the chance constraints is approximated in two different ways by a family of differentiable functions. This leads to two smooth parametric optimization problems IA_τ and OA_τ, where the feasible sets of IA_τ are always subsets (inner approximation) and the feasible sets of OA_τ always supersets (outer approximation). The feasible sets of IA_τ (resp. OA_τ) converge asymptotically to the feasible set of the CCPDE. Moreover, any limit point of a sequence of optimal solutions of IA_τ (resp. OA_τ) is a stationary point of CCPDE. The viability of the approximation approach is numerically demonstrated by optimal thermal cancer treatment as a case study.

Keywords: Chance constrained optimization, parabolic PDEs, smoothing approximation

1. INTRODUCTION

Partial differential equations are widely used to describe the spatial variations of the behaviors of physical, biological, social systems as well as processes in nature, industrial manufacturing, etc. In general, practical PDE models involve uncertainties arising from imprecise model parameters and the operational environment of the system. Frequently, a PDE model contains parameters, for example, describing heat capacity, diffusion, viscosity, hydraulic conductivity, pressure, permeability, etc. These parameters are usually difficult to precisely determine, i.e., they vary randomly in space and time. Therefore, the random parameters can be considered as *random fields*[1]-[11]. In real-life applications, external influences have a non-negligible impact and seriously disturb the system behavior. For example, ambient temperature and pressure are external uncertain influences imposing a serious impact on the performance of a PDE system. This means that such uncertainties will definitely cause significant uncertainties in state variables, thus leading to difficulties in dealing with their inequality constraints for optimization. Therefore, stochastic optimization methods are needed to gain optimal as well as reliable solutions for systems governed by PDEs under uncertainty.

This work considers uncertain influences arising from model parameters (coefficients), forcing term, and boundary conditions of PDE systems and assumes that all uncertain influences are random variables. As a result, we study the chance constrained optimization of boundary-value parabolic PDE systems (CCPDE), where chance constraints are imposed on the inequality constraints involving state variables. Preliminary theoretical functional space analysis of elliptic CCPDE problems can be found in our recently work [7]. Recently the work [6; 7; 14] (also related work [13]) study chance constrained optimization problems on infinite dimensional spaces. Nevertheless, solution approaches for CCPDE problems are not yet well-developed. Hence, this work demonstrates the practical applicability of the approach developed in [7] for the solution of CCPDE problems with parabolic PDE systems. Moreover, as a case-study, we consider chance constrained optimal control of a parabolic PDE system that naturally arises in hyperthermia treatment (HT)[2; 3; 5; 12]. It is now a well established practice to use HT as a pretreatment strategy in modern clinical cancer therapy.

The numerical computation of CCPDE needs a finite dimensional representation through space-time discretization coupled with appropriate sampling for the random variables. Since the resulting finite dimensional chance constrained optimization problem is generally nonsmooth, nonconvex and are difficult to solve directly, we use our recently proposed smoothing inner-outer approximation approach [9; 7] for the solution of the CCPDE problem.

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The paper is organized as follows. Section 2 presents the problem definition of CCPDE. Section 3 discusses basic concepts and relevant results of the inner-outer approximation approach. Section 4 presents a hypothetical hyperthermia treatment problem as a case study. The problem is modeled as a CCPDE problem and subsequently solved through the inner-outer approximation approach after an appropriate finite dimensional discretization. Finally, the study concludes with Section 5 by providing summary and future work.

2. PROBLEM DEFINITION

We consider the following optimal control problem of parabolic PDE systems under random data (CCPDE)

$$\min_u J(u) = E[\|T - T_d\|]^2_{H^1_g(D,[t_0,t_f])} + \frac{\gamma}{2}\|u\|^2_{L^2(D,[t_0,t_f])} \quad (1)$$

subject to:

$$\frac{\partial T}{\partial t} - \nabla.[\kappa(\xi_1, t, x)\nabla T)]$$

$$= Q(\xi_2, t, x), \text{ for } (t, x) \in [t_0, t_f] \times D, \xi \in \Omega \text{a.s.}; \quad (2)$$

$$T = g(u, \xi_3, t, x), \text{ for } (t, x) \in [t_0, t_f] \times \partial D, \xi \in \Omega \text{ a.s.}; \quad (3)$$

$$T(x, t_0) = T_0(x), \text{ for } x \in D; \quad (4)$$

$$Pr\{T_{min} \leq T(u, \xi, t, x) \leq T_{max}\} \geq \alpha; \quad (5)$$

$$u_{min} \leq u(t, x) \leq u_{max}, \quad (6)$$

where $D \subset \mathbb{R}^n$ $(n = 1, 2, 3)$ is bounded spatial domain with Lipschitz boundary ∂D; $x \in D$ represents the spatial variables; $\xi = (\xi_1, \xi_2, \xi_3) \in \Omega \subset \mathbb{R}^p$ is a vector of random input variables from a probability space $(\Omega, \mathcal{F}, \mathcal{P})$, $\mathcal{F}$ is the σ-algebra and $\mathcal{P}$ is a probability measure with a probability density function $\phi(\xi)$ associated to ξ; the interval $[t_0, t_f]$ represents the optimization time-horizon.

The parabolic PDE system (2) with Drichlet boundary (3) condition and initial value (4) represents a distributed control system. The coefficient $\kappa(\xi_1, t, x)$ is a random field, where ξ_1 represents the random inputs due to model parameter uncertainties. The system is driven by a distributed random forcing term $Q(u, \xi_2, t)$, where ξ_2 stands for random input uncertainties, i.e., due to errors in measurement devices. The boundary condition (3) specifies a boundary value $g(u, \xi_3, t, x)$ for the states T with ξ_3 representing random external influences that act through the boundary ∂D at the time instant $t \in [t_0, t_f]$. Due to the various random influences $\xi = (\xi_1, \xi_2, \xi_3)$, the state T is a random variable and also depends on the control u which is indicated by $T(u, \xi; t, x)$. Hence, it is assumed that $T(u, \cdot; t, \cdot) \in L^p(\Omega; \mathcal{V}), V = H^1_g(D))$, where $\mathcal{V} = H^1_g(D)$ is a Banach space, e.g., $\mathcal{W} = L^2(\Omega, H^1_g(D))$ or $\mathcal{W} = L^2(\Omega \times H^1_g(D))$, and $\|T(u, \cdot; t, \cdot)\|^p_{L^p(\Omega;\mathcal{V})} = \int_\Omega \left[\int_D |T(u, \xi; t, x)|^p \, dx\right] \phi(\xi) d\xi$ $+ \int_\Omega \left[\int_{\partial D} |\nabla T(u, \xi; t, x)|^p \, ds\right] \phi(\xi) d\xi = E\left[\|T(u, \xi; t, \cdot)\|^p_{\mathcal{V}}\right] < \infty$ for each $t \in [t_0, t_f]$; u represents the controls and $u(t, \cdot) \in \mathcal{U} = \{v \in L^2(D) | \ u_{min} \leq v \leq u_{max}, v \in \mathbb{R}^m\}$. In general, the control variables u are deterministic.

The operators $E[\cdot]$ and $Pr(\cdot)$, respectively, represent the expected value and probability measure with respect to the random variables ξ. The constraint in equation (5)

$$Pr\{T_{min} \leq T(u, \xi; t, x) \leq T_{max}\} \geq \alpha$$

specifies the probability (reliability) of holding restrictions on the state variable, where $\alpha \in [0, 1]$ is a pre-specified level of reliability. Hence, the chance constraint (5) is required to hold *point-wise* over the spatial domain D at each time instant $t \in [t_0, t_f]$.

The purpose of the control is to optimally attain a desired temperature profile T_d as accurately as possible, despite all random influences. The constant $\gamma > 0$ is a regularization parameter for the energy or cost term $\|u(t, \cdot)\|_{L^2(D)}$.

Associated to the chance constraint of CCPDE, we have the function

$$p(u; t, x) = Pr\{T_{min} \leq T(u, \xi; t, x) \leq T_{max}\} \quad (7)$$

which is commonly known as the *probability function* of the chance constraint (5), where $p(\cdot; t, x) : U \to [0, 1]$, for each fixed $(t, x) \in [t_0, t_f] \times D$. Subsequently, the feasible set of the CCPDE is represented by

$$\mathcal{P} = \{u \in U \mid p(u; t, x) \geq \alpha, (t, x) \in [t_0, t_f] \times D\}. \quad (8)$$

In general, the mathematical analysis of this problem demands relevant function spaces, specifically Sobolev and Bochner spaces.

3. SMOOTHING INNER-OUTER APPROXIMATION METHODS

For the sake of brevity, we assume that for a given $u \in U$ and a realization of the random variable $\xi \in \Omega$, there is a unique weak solution of the PDE system given by $T(u, \xi; t, x)$ [1]. Accordingly the problem CCPDE can be stated in a reduced form as follows

$$(CCPDE_{reduced}) \min_u \ J(u) \quad (9)$$

subject to:

$$Pr\{T_{min} \leq T(u, \xi; t, x) \leq T_{max}\} \geq \alpha \quad (10)$$

$$(t, x) \in D \times [t_0, t_f]$$

$$u \in U \quad . \quad (11)$$

The major computational bottleneck comes from the non-smoothness and above all, from the difficulty to evaluate the chance constraint of CCPDE. Based on our inner-outer approximation approach [7; 8] we use computationally amenable smoothing approximations of CCPDE in order to attain approximate solutions.

To guarantee that the problem posses fair mathematical properties, it is commonly necessary to assume that the set of random variables $\{\xi \in \Omega \mid T = T_{min} \text{ or } T = T_{max}\}$ to be of measure zero. This is commonly known as *measure zero property*. Briefly, the smoothing approximations are based on the following essential equivalent representations of probability functions $p(u) = Pr\left\{\hat{T}(u, \xi; t, x) \leq 0\right\} \geq \alpha$ $\equiv 1 - Pr\left\{\hat{T}(u, \xi; t, x) \geq 0\right\} \leq 1 - \alpha$, where $\hat{T}(u, \xi; t, x) = T - T_{max} \leq 0$ or $T_{min} - T \leq 0$. By using the upper semi-continuous Heaveside(unit jump) function

$$h(s) = \begin{cases} 1, \text{ if } s \geq 0, \\ 0, \text{ if } s < 0. \end{cases}$$

[1] This claim can be substantiated through a standard functional analytic argument using the Lax-Milgram Theorem.

The following well-known identities are obtained

$$p(u;t,x) = E[h(-\hat{T}(u,\xi;t,x))] = 1 - E[h(\hat{T}(u,\xi;t,x))] \quad (12)$$

where

$$E[h(\hat{T}(u,\xi;t,x))] = \int_{\Omega} \hat{T}(u,\xi;t,x)\phi(\xi)d\xi.$$

Despite the appealing expected value representation of probability functions in (12), the missing smoothness of the unit jump function does not provide computational advantages. Nevertheless, the function h provides an insight for the construction of a smoothing approximation for the probability function p. Hence, for $h(s)$ and $h(-s)$, the approach [7; 8] uses smoothing approximating scalar functions defined by introducing the parametric function

$$\Theta(\tau,s) = \frac{1+m_1\tau}{1+m_2\tau\exp\left(-\frac{s}{\tau}\right)}, \quad for \;\; \tau \in (0,1), \; s \in \mathbb{R}, \quad (13)$$

with the parametric family $\{\Theta(\tau,\cdot), \tau \in (0,1)\}$ of functions $\Theta : (0,1) \times \mathbb{R} \rightarrow \mathbb{R}_+$ possessing the following *strict monotonicity* and *uniform limit* properties:

P1: There is a constant C with $1 < C < +\infty$ such that
$$C \geq \Theta(\tau,s) > h(s), \forall s \in \mathbb{R}, \tau \in (0,1). \quad (14)$$
P2: $\Theta(\cdot,s)$ is strictly increasing on $(0,1)$, for each $s \in \mathbb{R}$,
P3: $\Theta(\tau,\cdot)$ is continuously differentiable and strictly increasing on $\mathbb{R}$, for each $\tau \in (0,1)$,
P4: $\inf_{\tau\in(0,1)} \Theta(\tau,s) = h(s)$, for all $s \in \mathbb{R}$,
P5: $\lim_{\tau\searrow 0_+} \sup_{s\in(-\infty,-\varepsilon)\cup[0,\infty)}(\Theta(\tau,s) - h(s)) = 0$, for all $\varepsilon > 0$.

Now, based on the parametric function Θ the following functions are defined $\psi(\tau,u;t,x) := E\left[\Theta(\tau,\hat{T}(u,\xi;t,x))\right]$ and $\varphi(\tau,u;t,x) := E\left[\Theta(\tau,-\hat{T}(u,\xi;t,x))\right], \tau \in (0,1)$. Under the measure zero property and smoothness properties of $\hat{T}(u,\xi;t,x)$, the functions $\psi(\tau,u;t,x)$ and $\varphi(\tau,u;t,x)$ can be shown to be smoothing approximations of $1 - p(u;t,x)$ and $p(u;t,x)$, respectively (see Geletu etal.[7]). Moreover, the following convergence properties

$$\inf_{\tau\in(0,1)} \varphi(\tau,u;t,x) = p(u;t,x) \quad (15)$$

$$\sup_{\tau\in(0,1)} (\psi(\tau,u;t,x)) = 1 - p(u;t,x) \quad (16)$$

and dominance properties
$1 - p(u;t,x) \leq \psi(\tau,u;t,x) \leq 1-\alpha$
$\varphi(\tau,u;t,x) \geq p(u;t,x) \geq \alpha$, for $(t,x) \in [t_0,t_f] \times D$
hold true. Now, using the parametric functions $\psi(\tau,\cdot)$ and $\varphi(\tau,\cdot)$, we define the following problems with the same objective function J as in CCPDE.

$\min_u J(u) \quad (IA_\tau)$	$\min_u J(u) \quad (OA_\tau)$
s.t. $\psi(\tau,u;t,x) \leq 1-\alpha, x \in D_c$, $u \in U$,	s.t. $\varphi(\tau,u;t,x) \geq \alpha$, $u \in U$,

with respective feasible sets

$$\mathcal{M}(\tau) := \{u \in U \mid \psi(\tau,u;t,x) \leq 1-\alpha, (t,x) \in [t_0,t_f] \times D\},$$
$$\mathcal{S}(\tau) := \{u \in U \mid \varphi(\tau,u;t,,x) \geq \alpha, (t,x) \in [t_0,t_f] \times D\}.$$

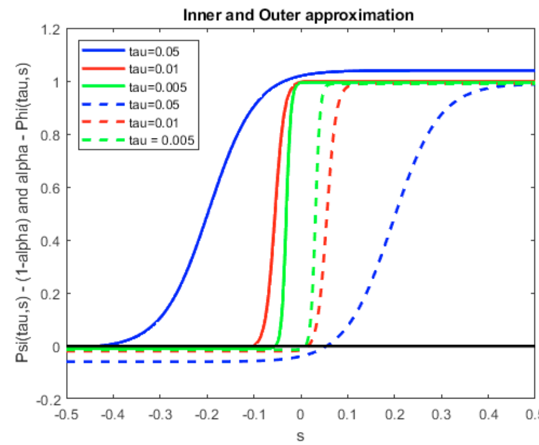

Fig. 1. Plot of $\theta(\tau,s), \theta(\tau,-s)$ versus s

As a consequence of the properties of the functions $\psi(\tau,u;t,x)$ and $\varphi(\tau,u;t,x)$ we have the following relations among the feasible sets of CCPDE, IA_τ and OA_τ. That is

$$M(\tau) \subset \mathcal{P} \subset S(\tau), \;\text{for}\; \tau \in (0,1).$$

which implies that the feasible sets $M(\tau)$ of IA_τ are always subsets of the feasible set $\mathcal{P}$ of CCPDE, while the feasible sets $S(\tau)$ of OA_τ are always supersets of the feasible set $\mathcal{P}$ of CCPDE. Furthermore, under the relevant assumptions, the following can be shown [7; 8]:

A) the sets $\mathcal{M}(\tau)$ and $\mathcal{S}(\tau)$ are closed, for each $\tau \in (0,1)$.
B) For $0 < \tau_2 \leq \tau_1 < 1$, the following inclusions hold
$$\mathcal{M}(\tau_1,x) \subset \mathcal{M}(\tau_2) \subset \mathcal{P}(x) \subset \mathcal{S}(\tau_2,x) \subset \mathcal{S}(\tau_1). \quad (17)$$
C)
$$\bigcap_{\tau\in(0,1)} \mathcal{S}(\tau) = \mathcal{P}. \quad (18)$$
D)
$$cl\left(\bigcup_{\tau\in(0,1)} \mathcal{M}(\tau)\right) = \mathcal{P}. \quad (19)$$

With the above properties, the solutions of the IA_τ are always feasible to CCPDE and the solutions of CCPDE are always feasible to OA_τ. Above all, any limit-point of a sequence of optimal solutions of IA_τ (resp. OA_τ) is a stationary point of CCPDE [7; 8]. Consequently, instead of solving the difficult CCPDE problem directly, we solve the relatively simpler smooth optimization problems IA_τ and OA_τ, respectively, for a selected decreasing sequence of parameters $\{\tau_k\} \in (0,1)$. Numerically, a good approximate solution to the CCPDE is said to be found if, for some parameter τ_k, the corresponding optimal objective functions values $J(u^*_{IA}(\tau_k))$ and $J(u^*_{OA}(\tau_k))$ are sufficiently close.

4. A CASE STUDY

Hyperthermia treatment (HT) and planning is used as an accompanying strategy in modern clinical cancer therapy[5]. Hyperthermia treatment consists in the heating of a tumor tissue in order to subdue or eradicate the growth of tumor cells from a given organ. The procedure of HT aims at heating tumor to a given temperature without causing damage on the healthy surrounding tissue due to overheating.

The heating is usually done through multiple electromagnetic (EM) sources, where each EM source generates an electric field $G(x)$ with a heat capacity c, density ρ, the phases and amplitude p. As a result, the electric fields facilitate a net power deposition on the tumor region given by [5] (e.g. $Q(x) = \frac{\sigma(\xi)}{2}|G(x)|^2$,where $G(x) = \sum_{j=1}^{N} p_j G_j x$ is a linear superposition of the individual fields and $\sigma(x)$ is the electric conductivity. In general, the phases and the power Q, corresponding to each individual antenna, are not known in advance.

The Mathematical model: Pennes bioheat [11] equation

$$\rho \cdot c_t \cdot \frac{\partial T}{\partial t} - div\,(\kappa \nabla T) + \omega \cdot c_b \cdot (T - T_a) = Q; \text{in}(t_0, t_f) \times D \quad (20)$$

is frequently used to compute the temperature distribution T in the heated domain considering the power distribution Q as an input, where D represents the part of the human body that is relevant for therapy. Here, T - Temperature, T_a - Arterial blood temperature, Q - Power deposition, ρ - Tissue density, c_t - Specific heat capacity of tissue, c_b - Specific heat capacity of blood, κ - Tissue thermal conductivity, t_0 is initial time, t_f is final time and ω - Perfusion of blood.

Source of uncertainty: Despite the wide use of equation (20) in the analysis, planning and control of hyperthermia treatment, its parameters are found not to be identical across all patients. One major reason for this lies in the variability of tissue properties among patients. Hence, most parameters in equation (20) display large variations from patient to patient [4; 12]. Furthermore, even for a single patient, pre-clinical laboratory experiments and measurements could not provide precise characterization of the parameters in (20), owing to variations in the patient's body makeup, variability in biological tissue properties of body organs (e.g., brain, lung or liver) under treatment, etc. Therefore, the model parameters $\rho, c_t, \kappa, \omega$ and c_b are known to be uncertain [12]. As a result of these uncertainties, the predicted values of temperature distribution $T(x)$ on the tumor as well as the amount of heat spilled to healthy neighboring tissues display uncertainties [1; 3].

Optimization problem: The objective is to provide optimal thermal dose strategy to keep the tumor region uniformly heated to a desired temperature T_d during the treatment. At the same time, the heat injection should satisfy the required temperature level with a high reliability by avoiding over-heating of the healthy neighboring tissues under all boundary conditions.

To demonstrate the viability of the inner-outer approximation approach, we study the following hypothetical HT problem [3].

$$\min_{u} E[\|T - T_d\|^2_{L^2(D)}] + \frac{\gamma}{2}\|u\|^2_{L^2(D)} \quad (21)$$

subject to:

$$\frac{\partial T}{\partial t} - \nabla(\kappa(x, \xi_1, t)\nabla T) + c_b \rho_b (T - T_b) = Q(x, \xi_2, t), \quad (22)$$

in $[t_0, t_f] \times D, \xi \in \Omega\ a.s.,$

$$T = g(u, \xi_3, x, t) \text{ on } U \times \Omega_3 \times \partial D, \quad (23)$$

$$Pr\{T(u, \xi, x, t) \le T_c = 2.999\} \ge \alpha, (x) \in D, \quad (24)$$

with

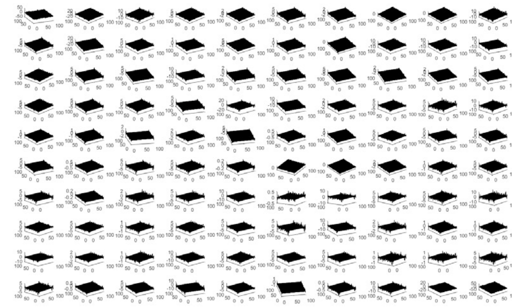

Fig. 2. Optimal state: surface temperature T with x decreasing in each descretized time

$$0 \le u \le 1, \quad (25)$$

$$\kappa(x, \xi_1) = 1, \quad (26)$$

$$Q(x, \xi_1) = \xi_1 exp(-sin(x_1)(x_1 + t)/(sin(t) + 4)) + 4sin(x_2)sin(t), \quad (27)$$

$$g(u, \xi_2, x) = (u(x) - T)\xi_2, \quad (28)$$

$$T_d = 40 - 2. * (x_1. * (x_1 - 1) + (x_2. * (x_2 - 1))), \quad (29)$$

$$\gamma = 10^{-3}, \alpha = 0.95, D = [0, 1] \times [0, 1], T(t_0 = 1) = 0, \quad (30)$$

$$T_{min} = 0, T_{max} = 40^0C. \quad (31)$$

The variables ξ_1, ξ_2, ξ_3 are standard normally distributed random variables. Samples for the random variables are generated by using the multi-level Monte Carlo (MLMC) sampling approach. Subsequently, at each step of the optimization algorithm, the PDE system is solved through the finite element method (FEM) by using a Matlab implementation. After discretization, the inner and outer approximation problems are solved using the Matlab optimization function **fmincon.m**, with each run decreasing values of $\tau = 10^{-k}, k = 1, \ldots, 5$ .The $IA \equiv OA$ a.s. as $\tau \to 0$ in Fig. 1.

Fig. 2 and Fig. 3 show the optimal temperature and control profiles for one hundred time steps in the treatment time horizon $[t_0, t_f] = [1, 100]$ (time in seconds). Fig. 4 to Fig. 8 show the error level between the controls of IA and OA for $\tau = 0.1$ to $\tau = 0.00001$, respectively, indicating that the errors will be decreased when the τ value is reduced. Fig. 9 displays the objective function of IA, OA and Error. The IA and the OA are converge uniformly at τ goes to zero from the right, in our case $\tau = 0.00001$.

Fig. 10 and Fig. 11 display magnifications of the optimal state temperature for time instant. The results of optimal state of IA and OA are shown in FIg. 10 for a fixed time $t = 50sec$, where $\tau = 10^{-5}$. Moreover, when τ is reduced to zero, the optimal controls of inner and outer approximation converge as indicated in Fig 8, the error is zero. The same case for the result of optimal control shows in Fig.12 with mesh generation that magnify plot functions in Fig. 2 $IA \equiv OA$ at $\tau = 0.00001$.

5. CONCLUSION AND FUTURE WORK

This study presents a computation approach to CCPDE problems and a preliminary investigation for optimal control of hyperthermia treatment of tumor tissues. Owing to the natural prevalence of uncertainties, the optimal

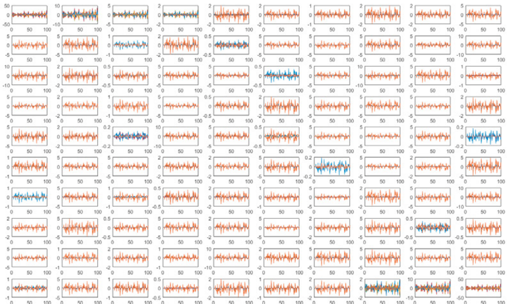

Fig. 3. control plot:surface temperature $u(x)$ decrease in t

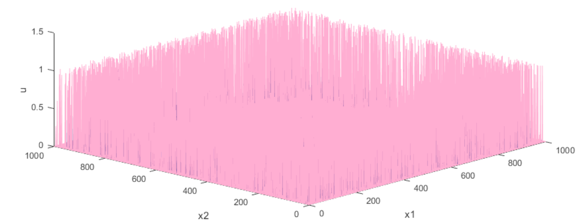

Fig. 4. Error at $\tau = 0.1$

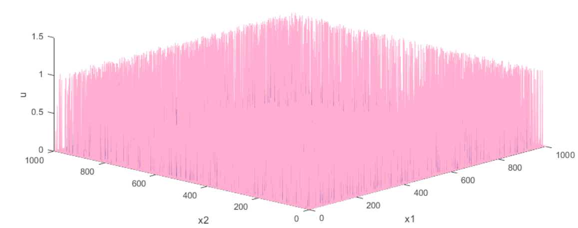

Fig. 5. Error at $\tau = 0.01$

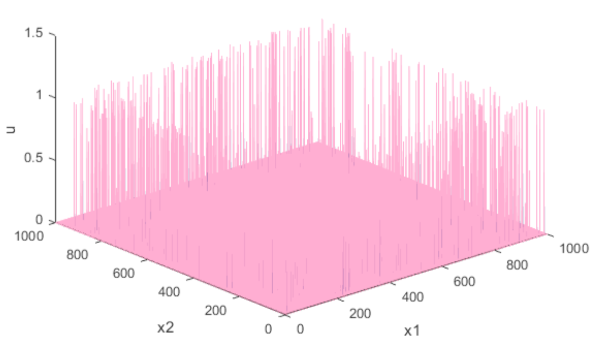

Fig. 6. Error at $\tau = 0.001$

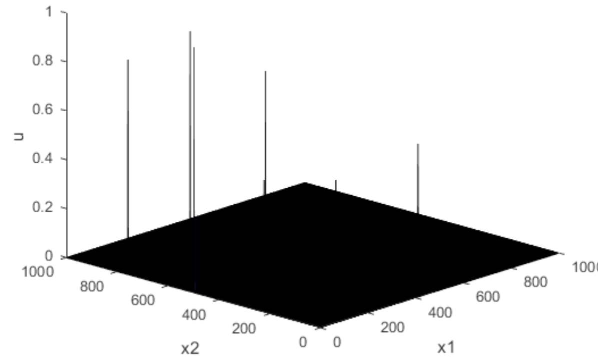

Fig. 7. Error at $\tau = 0.0001$

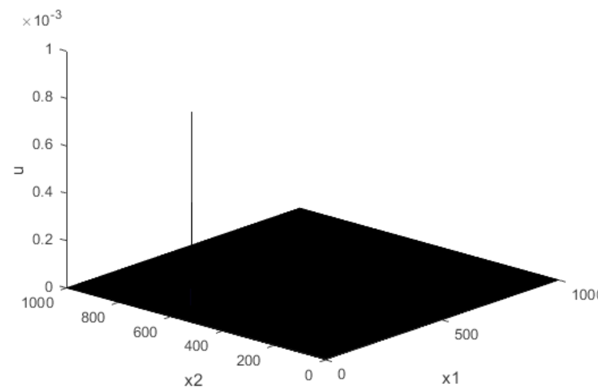

Fig. 8. Error at $\tau = 0.00001$

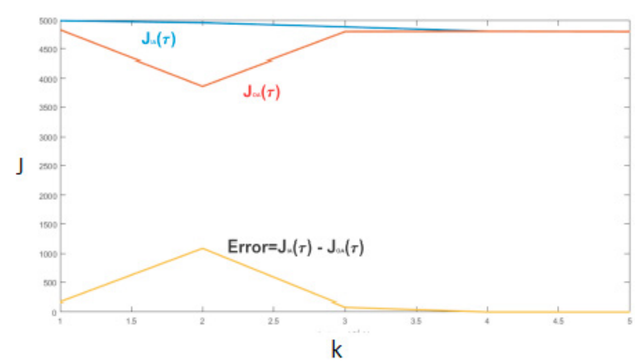

Fig. 9. Plot of objective function values $J_{IA}(\tau)$ and $J_{OA}(\tau)$, for $\tau = 10^{-k}$, k=1,. . . ,5.

bioheat treatment is modeled as a CCPDE problem. Subsequently, a hypothetical numerical example demonstrates that such a CCPDE problem can be effectively solved by the inner-outer approximation approach. A more realistic and concrete patient data-based consideration is left pending for future investigations. Moreover, tracking the desired temperature level for effective thermal dose

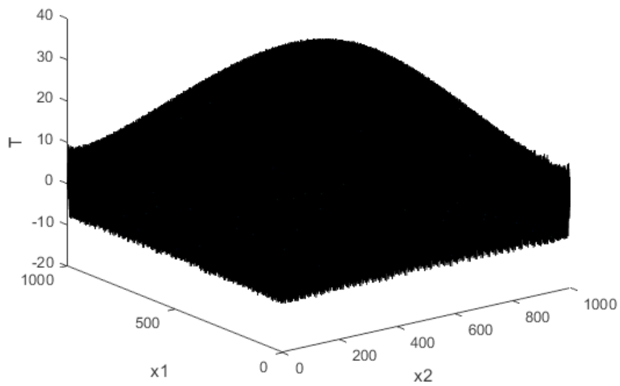

Fig. 10. surface of T that magnify each state in fig 1

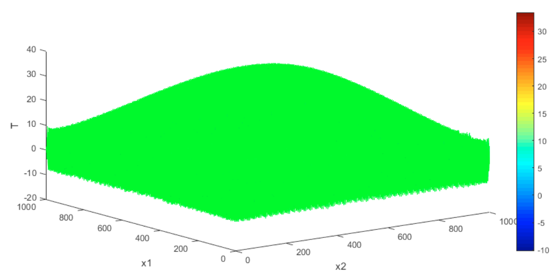

Fig. 11. surface of T w.r.t. x for fixed time

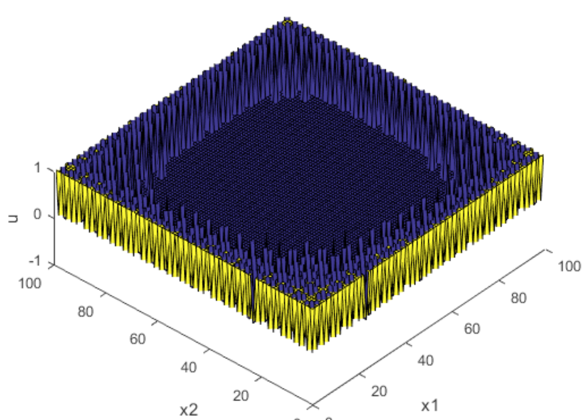

Fig. 12. The control u with mesh generation that magnify plot functions in fig 2 IA=OA at $\tau = 0.00001$

tumor treatment can be further studied using the model predictive control scheme.

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